76538

U.S. DEPARTMENT OF COMMERCE
Patent and Trademark Office

SEARCH REQUEST FORM

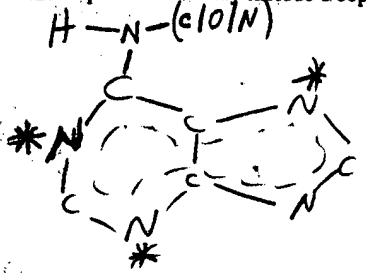
Requestor's Name: Bench

Serial Number: 09/740653

Date: 9-26-02 Phone: 4718

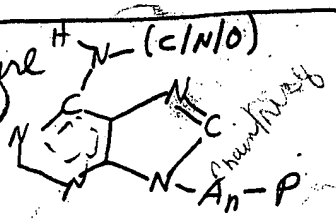
Art Unit: 1624
4D15 4E12

Search Topic:
Please write a detailed statement of search topic. Describe specifically as possible the subject matter to be searched. Define any terms that may have a special meaning. Give examples or relevent citations, authors, keywords, etc., if known. For sequences, please attach a copy of the sequence. You may include a copy of the broadest and/or most relevent claim(s).



MARY

With these requirements
1) Atoms marked with * cannot be further substituted
2) At least one P atom must be present
3) No multi-components (e.g. no salts)
4) exclude any compound of the type in Box

(A) Has structure 

not L18

A = any atom
n = 0-20
and (B) has exactly one P

Print all structures

MJ 1/8

1354
1335-45
53

BEST AVAILABLE COPY

STAFF USE ONLY

Date completed: 12/2
Searcher: Mary
Terminal time:
Elapsed time:
CPU time:
Total time: 49

Search Site
STIC
CM-1
Pre-S

Type of Search
N.A. Sequence

Vendors
IG
STN 12/1 11
Dialog
APS
Geninfo

Buch
740653

=> fil reg

COST IN U.S. DOLLARS	SINCE FILE ENTRY	TOTAL SESSION
FULL ESTIMATED COST	0.38	166.47

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)	SINCE FILE ENTRY	TOTAL SESSION
CA SUBSCRIBER PRICE	0.00	-3.54

FILE 'REGISTRY' ENTERED AT 13:35:38 ON 02 DEC 2002
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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
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Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 1 DEC 2002 HIGHEST RN 474745-06-7
DICTIONARY FILE UPDATES: 1 DEC 2002 HIGHEST RN 474745-06-7

TSCA INFORMATION NOW CURRENT THROUGH MAY 20, 2002

Please note that search-term pricing does apply when conducting SmartSELECT searches.

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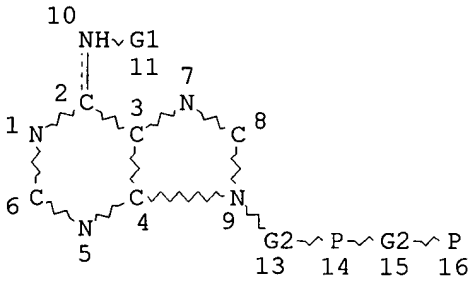
Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. See HELP PROPERTIES for more information. See STNote 27, Searching Properties in the CAS Registry File, for complete details:
http://www.cas.org/ONLINE/STN/STNOTES/stnotes27.pdf

=> d l18 que stat;d 1-20 ide cbib abs
L2 SCR 2127
L9 SCR 2017
L16 STR



VAR G1=C/O/N
REP G2=(0-20) A
NODE ATTRIBUTES:
CONNECT IS E2 RC AT 1
CONNECT IS E2 RC AT 5
CONNECT IS E2 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
L18 20 SEA FILE=REGISTRY SSS FUL L16 AND L9 NOT L2

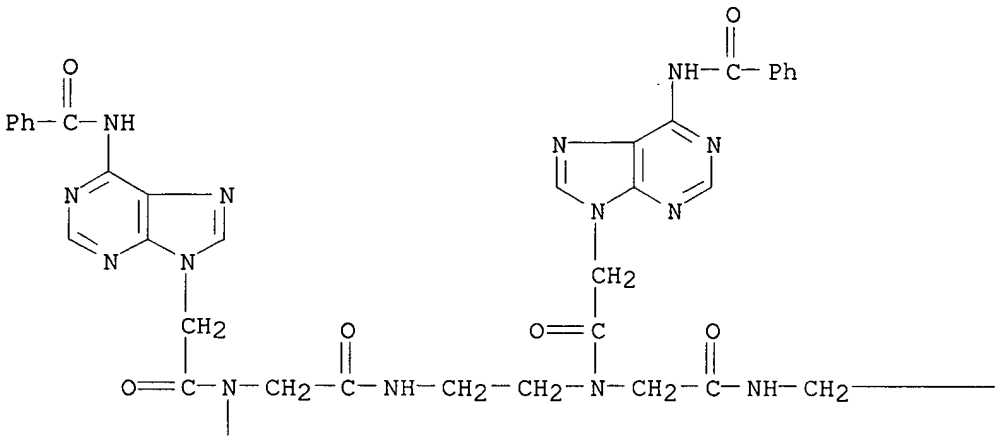
100.0% PROCESSED 4385 ITERATIONS 20 ANSWERS
SEARCH TIME: 00.00.02

L18 ANSWER 1 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 225787-02-0 REGISTRY
CN Peptide nucleic acid, ((deamino)(hydroxy)T-bz6A-bz6A-bz6A-bz6A)-Gly-OH, (4-carboxyphenyl)methyl ester, 5'-[2-cyanoethyl 4-[[(2-cyanoethoxy)(4-hydroxybutoxy)phosphinyl]oxy]butyl phosphate] (9CI) (CA INDEX NAME)
FS NUCLEIC ACID SEQUENCE
MF C107 H116 N34 O29 P2
SR CA
LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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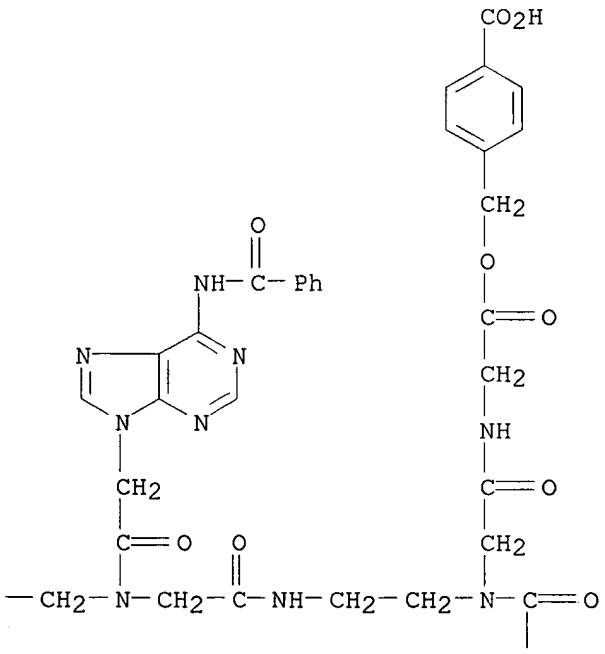

Searched by: Mary Hale 308-4258 CM-1 1E01

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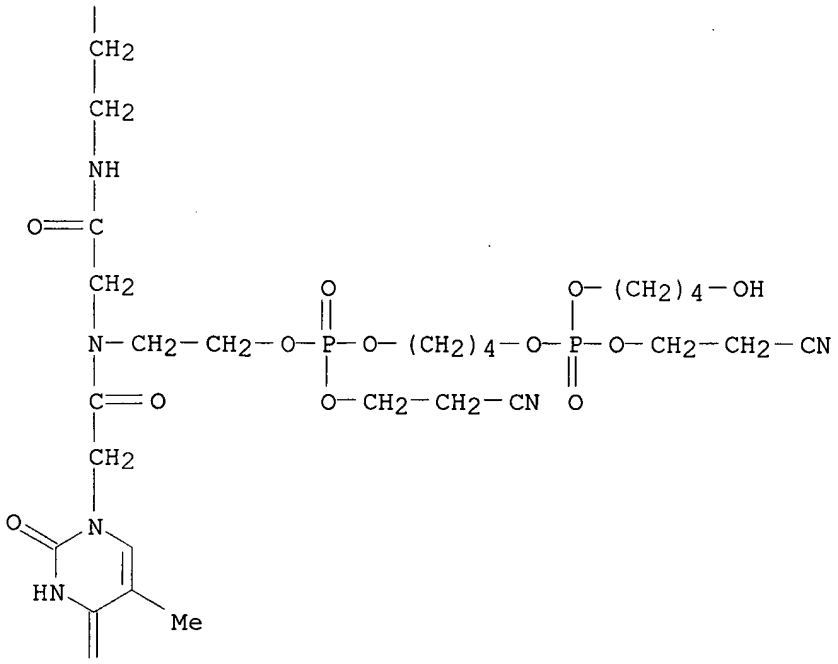

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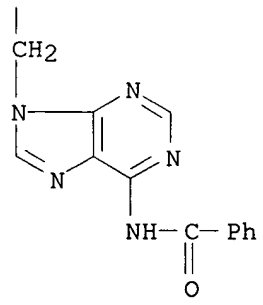


PAGE 3-A

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 131:19274 2',5'-oligoadenylate-peptide nucleic acids (2-5A-PNAs) activate RNase L. Verheijen, Jeroen C.; Van der Marel, Gijsbert A.; Van Boom, Jacques H.; Bayly, Suzanne F.; Player, Mark R.; Torrence, Paul F. (Gorlaeus Laboratories, Leiden Institute of Chemistry, Leiden, 2300 RA, Neth.). Bioorganic & Medicinal Chemistry, 7(3), 449-455 (English) 1999. CODEN: BMECEP. ISSN: 0968-0896. Publisher: Elsevier Science Ltd..

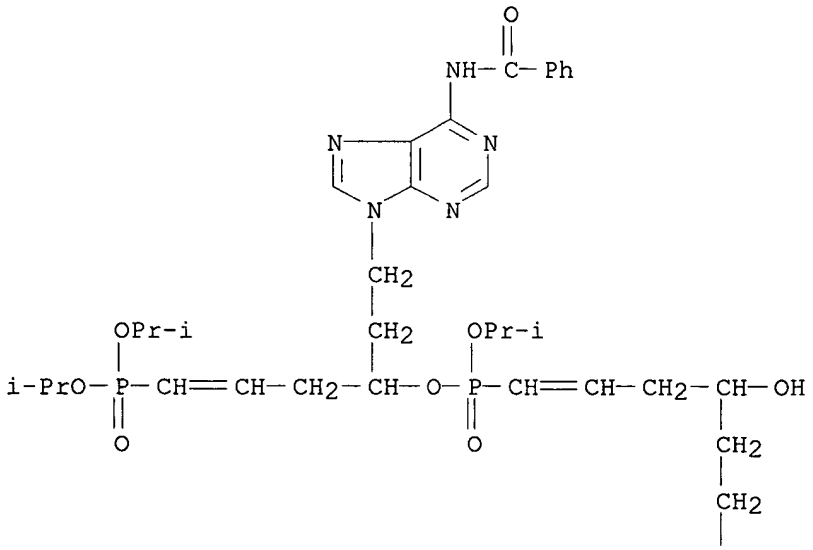
Searched by: Mary Hale 308-4258 CM-1 1E01

AB To potentiate the 2-5A (2',5'-oligoadenylate)-antisense and peptide nucleic acid (PNA) approaches to regulation of gene expression, composite mols. were generated contg. both 2-5A and PNA moieties. 2-5A-PNA adducts were synthesized using solid-phase techniques. Highly cross-linked polystyrene beads were functionalized with glycine tethered through a p-hydroxymethyl-benzoic acid linker and the PNA domain of the chimeric oligonucleotide analog was added by sequential elongation of the amino terminus with the monomethoxytrityl protected N-(2-aminoethyl)-N-(adenin-1-ylacetyl)glycinate. Transition to the 2-5A domain was accomplished by coupling of the PNA chain to dimethoxytrityl protected N-(2-hydroxyethyl)-N-(adenin-1-ylacetyl)glycinate. Finally, (2-cyanoethyl)-N,N-diisopropyl-4-O-(4,4-dimethoxytrityl)butyl-phosphoramidite and the corresponding (2-cyanoethyl)-N,N-diisopropylphosphoramidite of 5-O-(4,4'-dimethoxytrityl)-3-O-(tert-butyldimethylsilyl)-N6-benzoyl-adenosine were the synthons employed to add the 2 butanediol phosphate linkers and the four 2',5'-linked riboadenylates. The 5'-phosphate moiety was introduced with 2-[[2-(4,4'-dimethoxytrityloxy)ethyl]sulfonyl]ethyl-(2-cyanoethyl)-N,N-diisopropylphosphoramidite. Deprotection with methanolic NH3 and tetraethylammonium fluoride afforded the desired products, 2-5A-pnaA4, 2-5A-pnaA8 and 2-5A-pnaA12. When evaluated for their ability to cause the degrdn. of two different RNA substrates by the 2-5A-dependent RNase L, these new 2-5A-PNA conjugates were found to be potent RNase L activators. The union of 2-5A and PNA presents fresh opportunities to explore the biol. and therapeutic implications of these unique approaches to antisense.

L18 ANSWER 2 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 223409-57-2 REGISTRY
CN Phosphonic acid, [6-[6-(benzoylamino)-9H-purin-9-yl]-4-[[[6-[6-(benzoylamino)-9H-purin-9-yl]-4-hydroxy-1-hexenyl](1-methylethoxy)phosphinyl]oxy]-1-hexenyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)
FS 3D CONCORD
MF C45 H56 N10 O9 P2
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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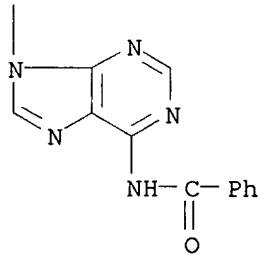

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 130:296947 Synthesis of acyclic carba-nucleoside phosphonates, structural analogs to natural deoxyribonucleotides. Esposito, Annamaria; Perino, Maria Grazia; Taddei, Maurizio (Dipartimento Chimica, Universita Sassari, Sassari, I-07100, Italy). European Journal of Organic Chemistry (4), 931-936 (English) 1999. CODEN: EJOCFK. ISSN: 1434-193X. Publisher: Wiley-VCH Verlag GmbH.

AB Acyclic carba-nucleoside phosphonates, modeled on natural deoxyribonucleotides were prepd. starting from DNA nucleobases and tert-Bu acrylate. The products obtained from a Michael-type reaction were elongated to .beta.-oxo esters that were first reduced to .beta.-hydroxy esters and then transformed into protected .beta.-hydroxy aldehydes. Wittig-Horner-Emmons reaction with the anion of CH2[PO(OCHMe2)2]2 gave,

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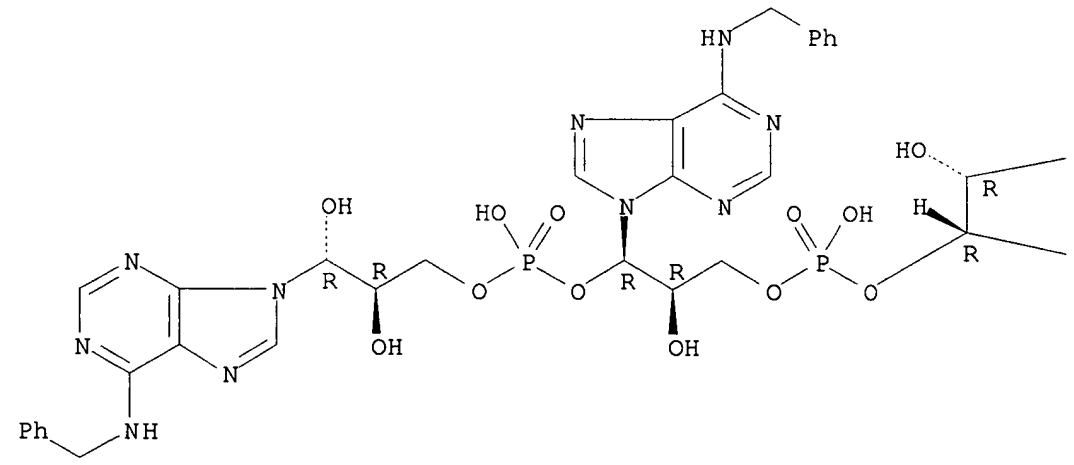
after deprotection, the desired 4-hydroxy-6-purinyl- or -6-pyrimidinyl-1-hexenylphosphonates. A dimer, potential precursor of acyclic polynucleotides (APN), homomorphous with DNA, was also prepd.

L18 ANSWER 3 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-23-1 REGISTRY
CN Phosphoric acid, mono[3-[[[2,3-dihydroxy-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propoxy]hydroxyphosphinyl]oxy]-2-hydroxy-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl] mono[2,3-dihydroxy-1-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl] ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C45 H49 N15 O13 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

PAGE 1-A



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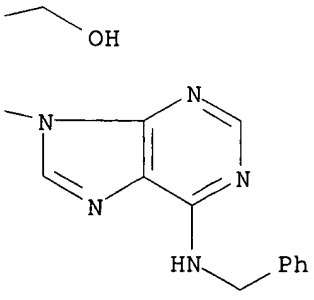


Searched by: Mary Hale 308-4258 CM-1 1E01

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

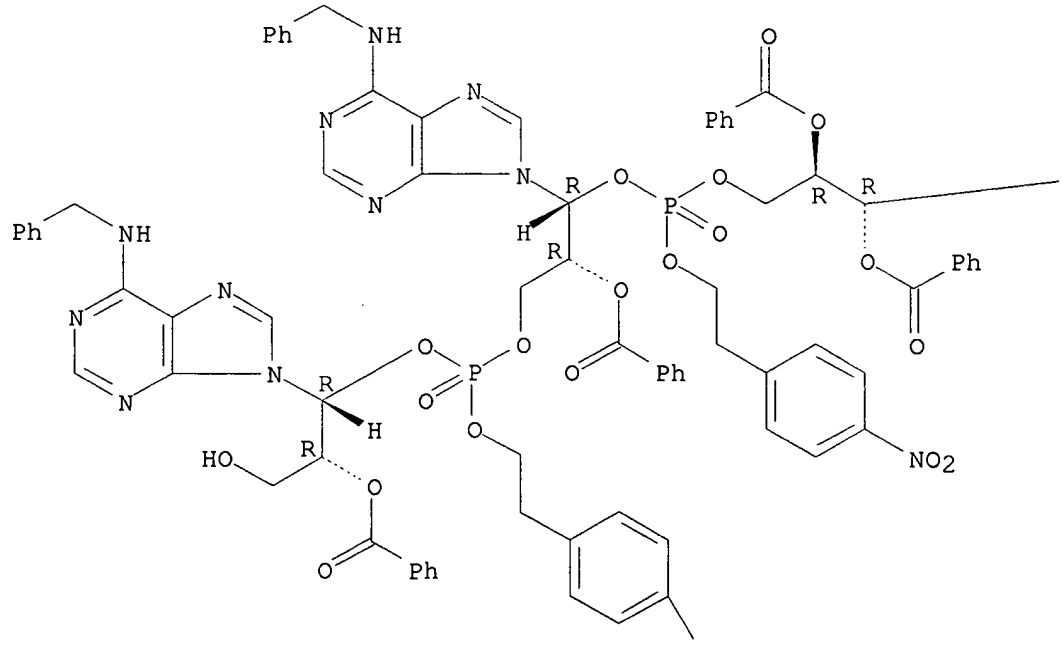
REFERENCE 1: 125:222336 N6-Benzyladenosine analogs of (A2'p)2A: synthesis and activity toward tobacco mosaic virus. Kvasyuk, E. I.; Kulak, T. I.; Zinchenko, A. I.; Barai, V. N.; Mikhailopulo, I. A. (Inst. Bioorg. Chem., Belaruss. Acad. Sci., Minsk, 220141, Belarus). Bioorganicheskaya Khimiya, 22(3), 208-214 (Russian) 1996. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.

AB Analogs of (2'-5')oligoadenylate trimer with N6-benzyladenosine in various positions of the chain and the fully substituted trimer were synthesized by the phosphotriester method. The structures of compds. prepd. were proved by UV, CD, and 1H NMR. The products inhibit replication of tobacco mosaic virus at 10-8-10-6 M, which is comparable to that of natural triadenylate (A2'p)2A.

L18 ANSWER 4 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-21-9 REGISTRY
CN Phosphoric acid, 2-(benzoyloxy)-3-[[[2,3-bis(benzoyloxy)-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propoxy][2-(4-nitrophenyl)ethoxy]phosphinyl]oxy]-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl 2-(benzoyloxy)-3-hydroxy-1-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl 2-(4-nitrophenyl)ethyl ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C89 H79 N17 O21 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

PAGE 1-A



Searched by: Mary Hale 308-4258 CM-1 1E01

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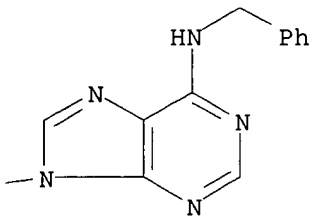

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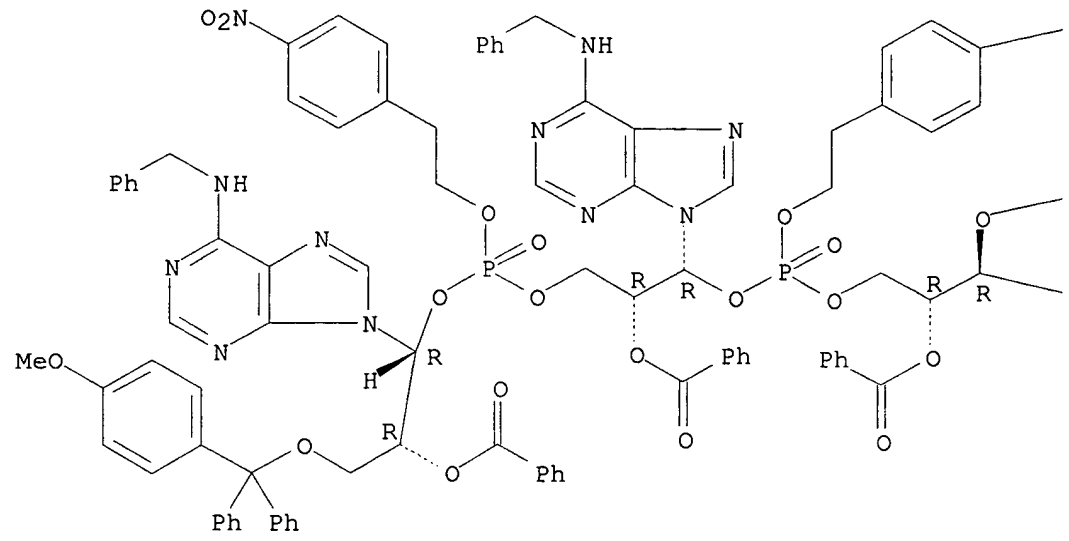
L18 ANSWER 5 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-19-5 REGISTRY
CN Phosphoric acid, 2-(benzoyloxy)-3-[[[2,3-bis(benzoyloxy)-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propoxy][2-(4-nitrophenyl)ethoxy]phosphinyl]oxy]-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl 2-(benzoyloxy)-3-[(4-methoxyphenyl)diphenylmethoxy]-1-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl 2-(4-nitrophenyl)ethyl ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C109 H95 N17 O22 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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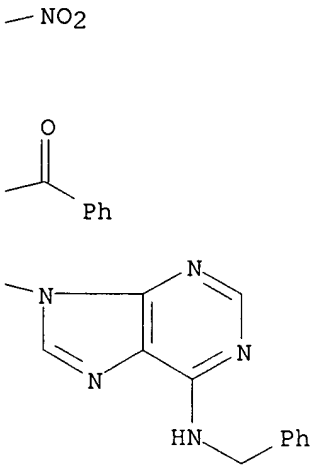

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L18 ANSWER 6 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-17-3 REGISTRY
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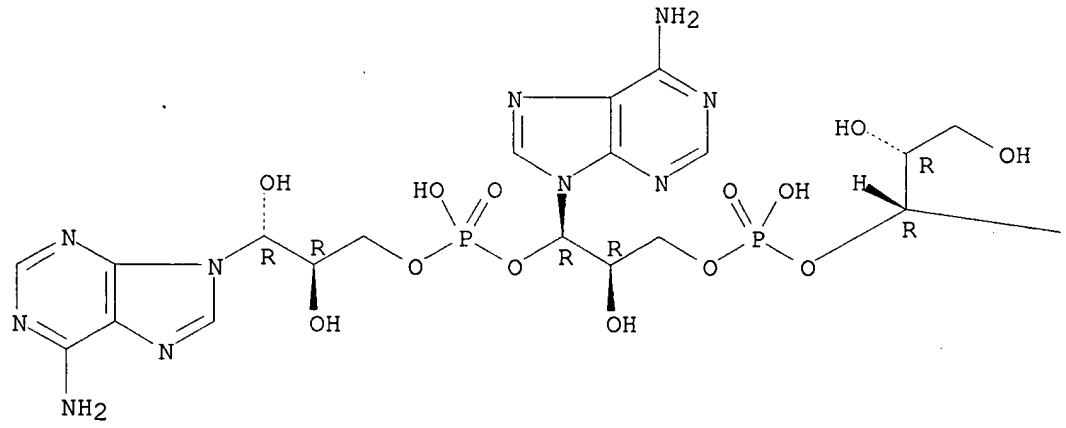
LC STN Files: CA, CAPLUS

Relative stereochemistry.

PAGE 1-A



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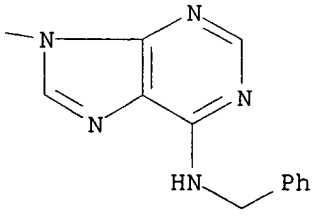

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L18 ANSWER 7 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-15-1 REGISTRY
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Relative stereochemistry.

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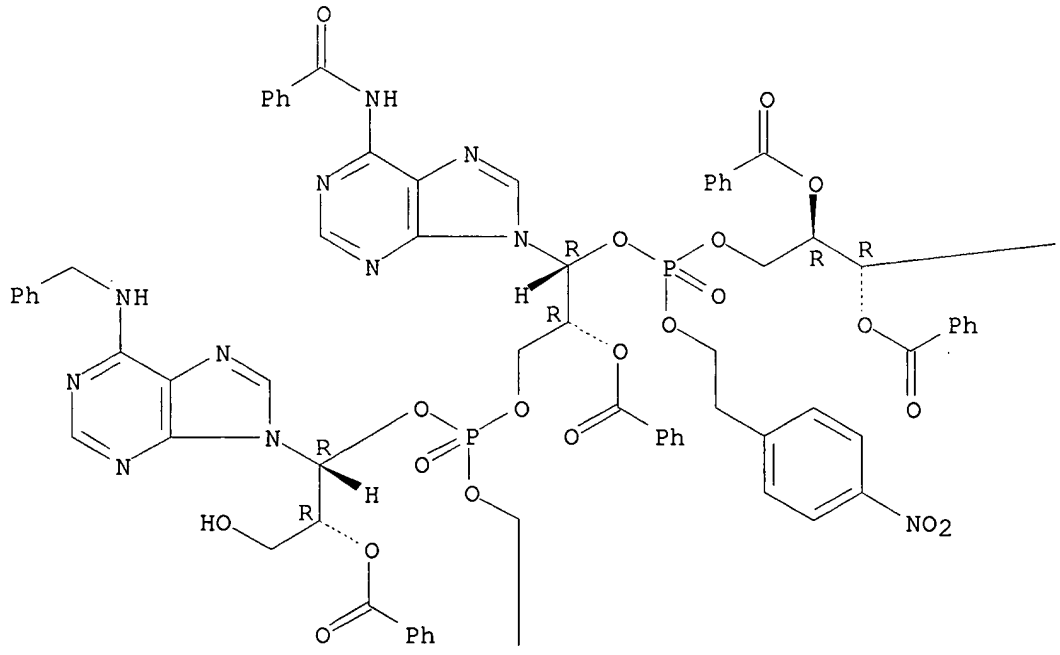

Searched by: Mary Hale 308-4258 CM-1 1E01

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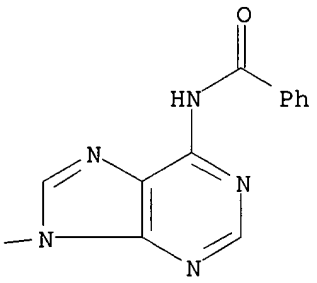

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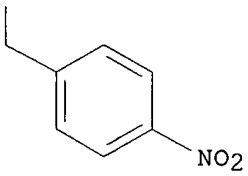

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1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:222336 N6-Benzyladenosine analogs of (A2'p)2A: synthesis and activity toward tobacco mosaic virus. Kvasyuk, E. I.; Kulak, T. I.; Zinchenko, A. I.; Barai, V. N.; Mikhailopulo, I. A. (Inst. Bioorg. Chem., Belaruss. Acad. Sci., Minsk, 220141, Belarus). Bioorganicheskaya Khimiya, 22(3), 208-214 (Russian) 1996. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.

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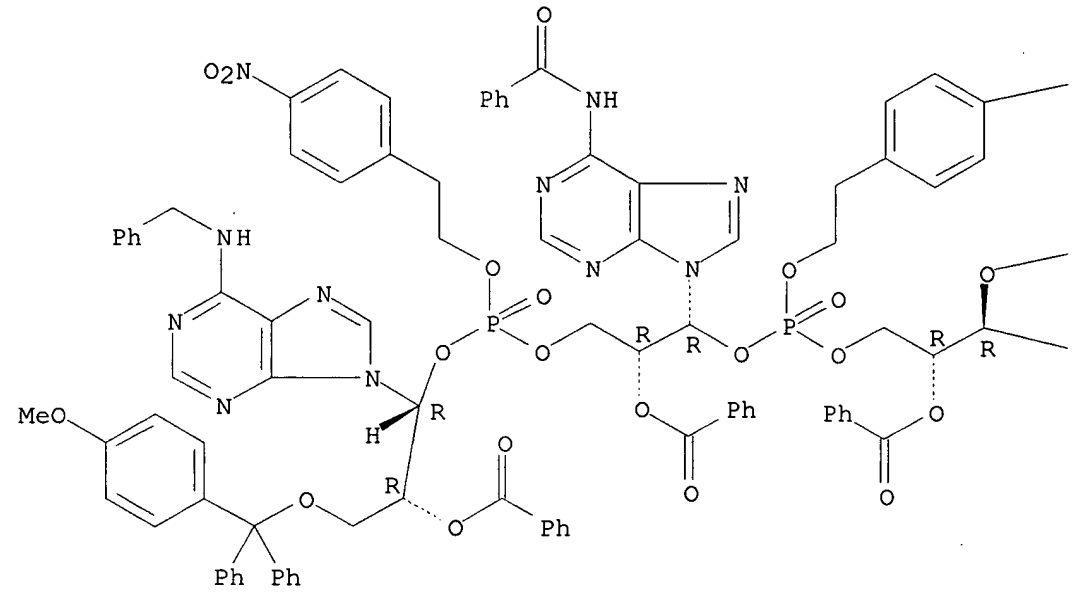
L18 ANSWER 8 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-13-9 REGISTRY
CN Phosphoric acid, 3-[6-(benzoylamino)-9H-purin-9-yl]-3-[[[3-[6-(benzoylamino)-9H-purin-9-yl]-2,3-bis(benzoyloxy)propoxy][2-(4-nitrophenyl)ethoxy]phosphinyl]oxy]-2-(benzoyloxy)propyl 2-(benzoyloxy)-3-[(4-methoxyphenyl)diphenylmethoxy]-1-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl 2-(4-nitrophenyl)ethyl ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C109 H91 N17 O24 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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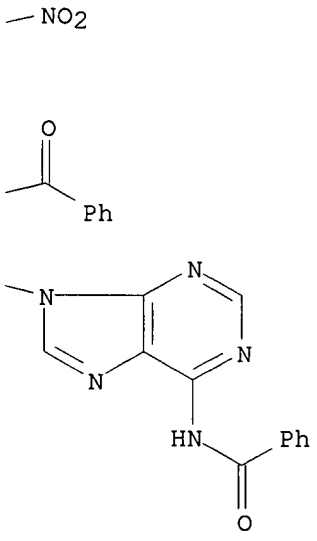

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:222336 N6-Benzyladenosine analogs of (A2'p)2A: synthesis and activity toward tobacco mosaic virus. Kvasyuk, E. I.; Kulak, T. I.;

Searched by: Mary Hale 308-4258 CM-1 1E01

Zinchenko, A. I.; Barai, V. N.; Mikhailopulo, I. A. (Inst. Bioorg. Chem., Belaruss. Acad. Sci., Minsk, 220141, Belarus). Bioorganicheskaya Khimiya, 22(3), 208-214 (Russian) 1996. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.

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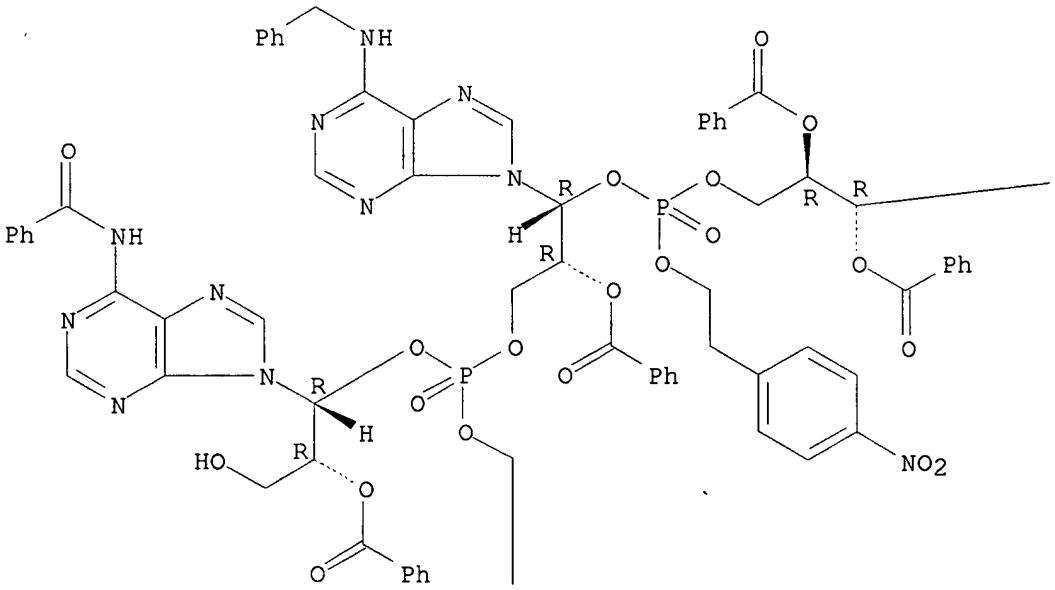
L18 ANSWER 9 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-10-6 REGISTRY
CN Phosphoric acid, 1-[6-(benzoylamino)-9H-purin-9-yl]-2-(benzoyloxy)-3-hydroxypropyl 3-[[[3-[6-(benzoylamino)-9H-purin-9-yl]-2,3-bis(benzoyloxy)propoxy][2-(4-nitrophenyl)ethoxy]phosphinyl]oxy]-2-(benzoyloxy)-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl 2-(4-nitrophenyl)ethyl ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C89 H75 N17 O23 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

PAGE 1-A



Searched by: Mary Hale 308-4258 CM-1 1E01

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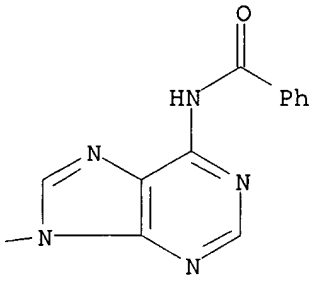

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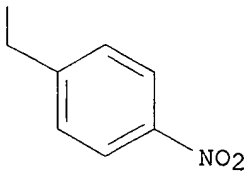

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 125:222336 N6-Benzyladenosine analogs of (A2'p)2A: synthesis and activity toward tobacco mosaic virus. Kvasyuk, E. I.; Kulak, T. I.; Zinchenko, A. I.; Barai, V. N.; Mikhailopulo, I. A. (Inst. Bioorg. Chem., Belaruss. Acad. Sci., Minsk, 220141, Belarus). Bioorganicheskaya Khimiya, 22(3), 208-214 (Russian) 1996. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.

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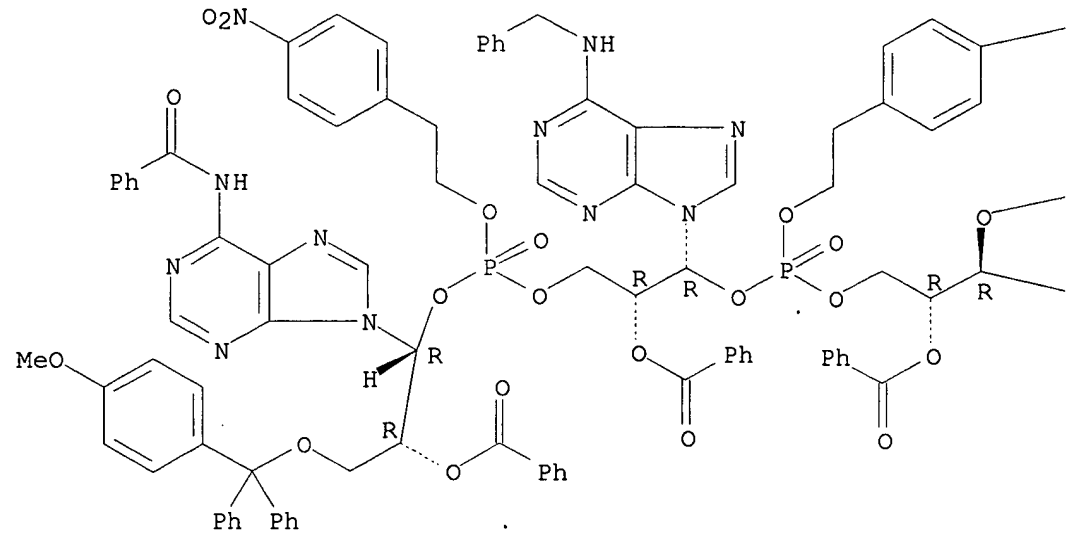
L18 ANSWER 10 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-08-2 REGISTRY
CN Phosphoric acid, 1-[6-(benzoylamino)-9H-purin-9-yl-2-(benzoyloxy)-3-[(4-methoxyphenyl)diphenylmethoxy]]propyl 3-[[[3-[6-(benzoylamino)-9H-purin-9-yl]-2,3-bis(benzoyloxy)propoxy][2-(4-nitrophenyl)ethoxy]phosphinyl]oxy]-2-(benzoyloxy)-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propyl 2-(4-nitrophenyl)ethyl ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C109 H91 N17 O24 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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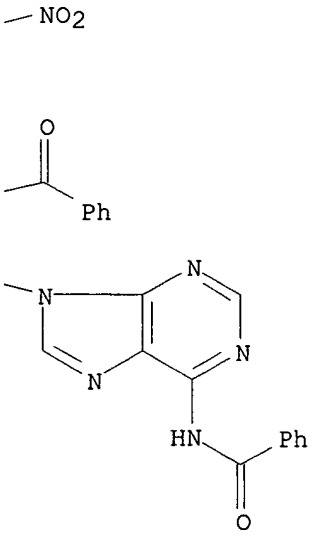

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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REFERENCE 1: 125:222336 N6-Benzyladenosine analogs of (A2'p)2A: synthesis and activity toward tobacco mosaic virus. Kvasyuk, E. I.; Kulak, T. I.; Zinchenko, A. I.; Barai, V. N.; Mikhailopulo, I. A. (Inst. Bioorg. Chem., Belaruss. Acad. Sci., Minsk, 220141, Belarus). Bioorganicheskaya Khimiya, 22(3), 208-214 (Russian) 1996. CODEN: BIKHD7. ISSN: 0132-3423. Publisher: MAIK Nauka.

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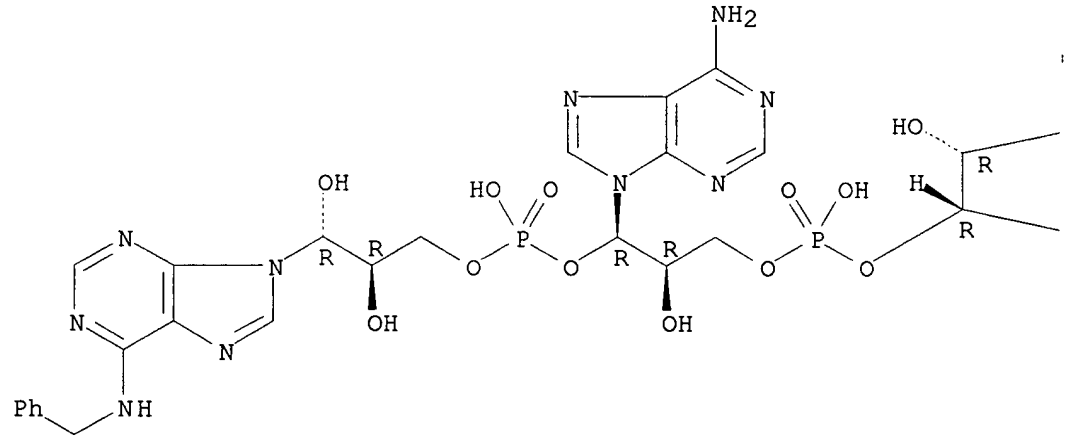
L18 ANSWER 11 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-06-0 REGISTRY
CN Phosphoric acid, mono[3-(6-amino-9H-purin-9-yl)-3-[[[2,3-dihydroxy-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propoxy]hydroxyphosphinyl]oxy]-2-hydroxypropyl] mono[1-(6-amino-9H-purin-9-yl)-2,3-dihydroxypropyl] ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C31 H37 N15 O13 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

PAGE 1-A



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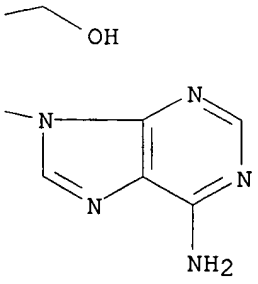

Searched by: Mary Hale 308-4258 CM-1 1E01

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

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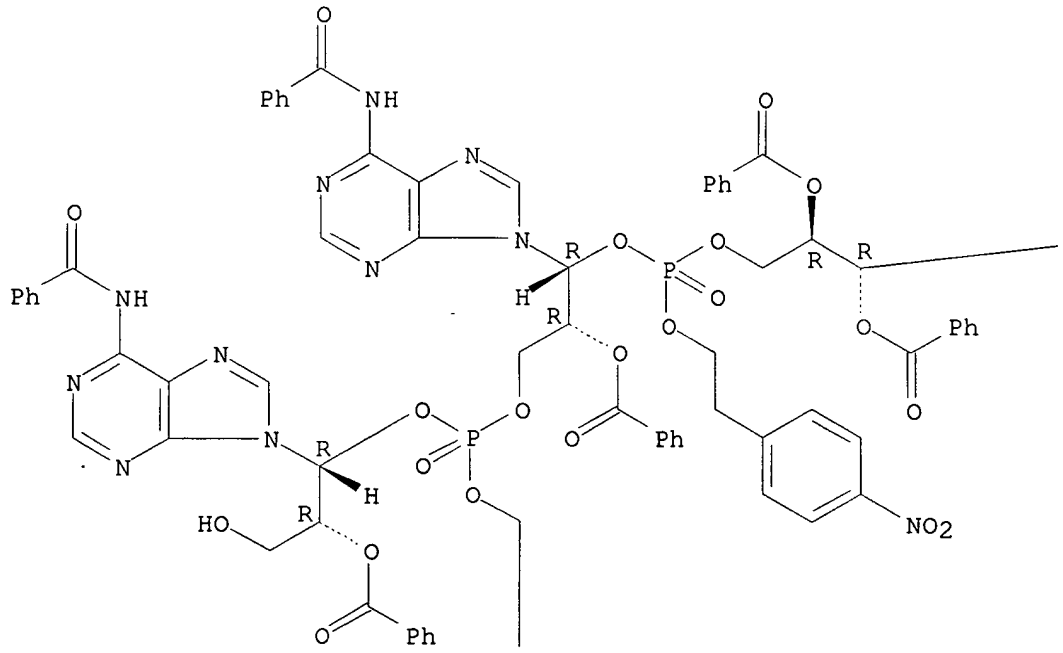
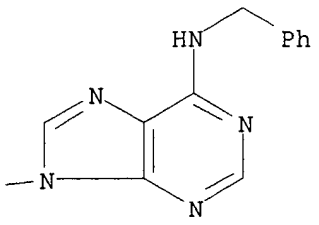
L18 ANSWER 12 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-04-8 REGISTRY
CN Phosphoric acid, 3-[6-(benzoylamino)-9H-purin-9-yl]-2-(benzoyloxy)-3-[[[2,3-bis(benzoyloxy)-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propoxy][2-(4-nitrophenyl)ethoxy]phosphinyl]oxy]propyl 1-[6-(benzoylamino)-9H-purin-9-yl]-2-(benzoyloxy)-3-hydroxypropyl 2-(4-nitrophenyl)ethyl ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C89 H75 N17 O23 P2
SR CA
LC STN Files: CA, CAPLUS

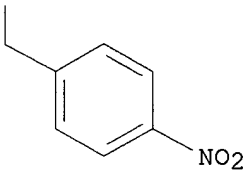
Relative stereochemistry.

PAGE 1-A



Searched by: Mary Hale 308-4258 CM-1 1E01





PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

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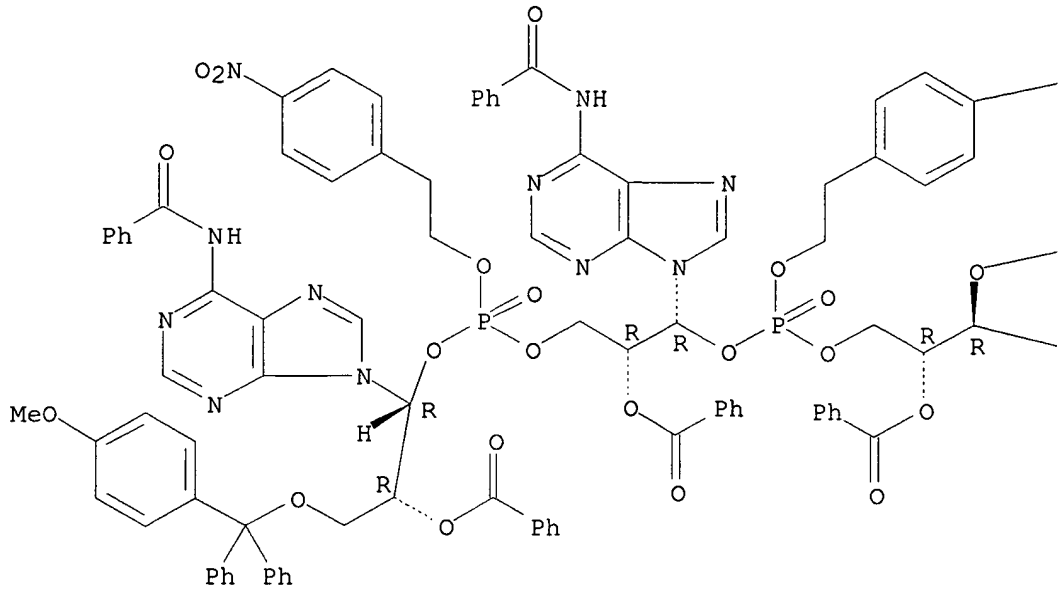
L18 ANSWER 13 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 181260-02-6 REGISTRY
CN Phosphoric acid, 3-[6-(benzoylamino)-9H-purin-9-yl]-2-(benzoyloxy)-3-[[[2,3-bis(benzoyloxy)-3-[6-[(phenylmethyl)amino]-9H-purin-9-yl]propoxy][2-(4-nitrophenyl)ethoxy]phosphinyl]oxy]propyl 1-[6-(benzoylamino)-9H-purin-9-yl]-2-(benzoyloxy)-3-[(4-methoxyphenyl)diphenylmethoxy]propyl 2-(4-nitrophenyl)ethyl ester, [1R*[2R*,3R*(2R*,3R*)],2R*]- (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C109 H91 N17 O24 P2
SR CA
LC STN Files: CA, CAPLUS

Relative stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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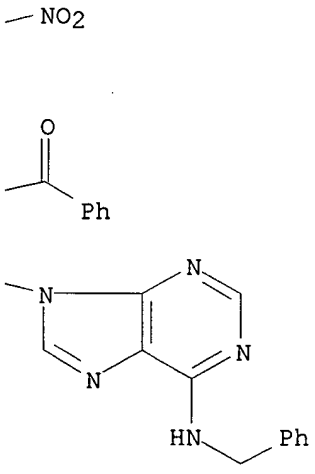

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

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Searched by: Mary Hale 308-4258 CM-1 1E01

22(3), 208-214 (Russian) 1996. CODEN: BIKHD7. ISSN: 0132-3423.
Publisher: MAIK Nauka.

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L18 ANSWER 14 OF 20 REGISTRY COPYRIGHT 2002 ACS

RN 173298-44-7 REGISTRY

CN Carbamimidic acid, [6-[[3-[[9-(1,3-diformyl-6,8,8-trihydroxy-6,8-dioxido-2,5,7-trioxa-6,8-diphosphaoct-1-yl)-9H-purin-6-yl]amino]-1-oxopropyl]amino]hexyl]- (9CI) (CA INDEX NAME)

OTHER CA INDEX NAMES:

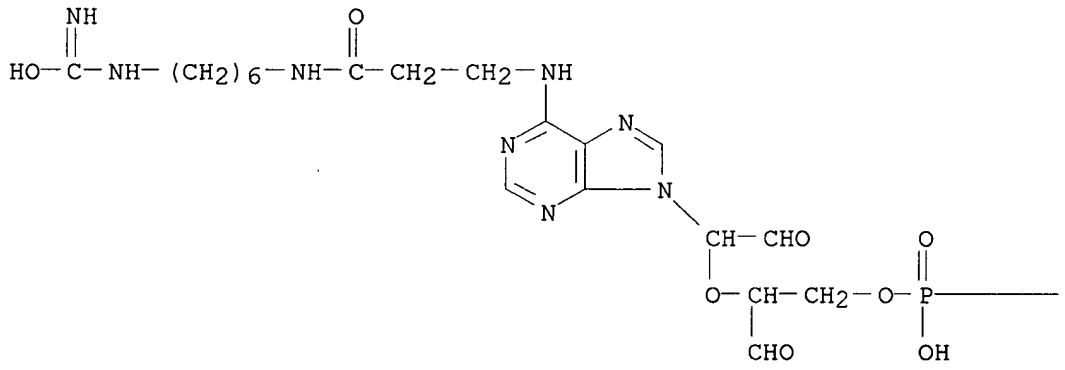
CN Carbamimidic acid, [6-[[3-[[9-(1,3-diformyl-6,8,8-trihydroxy-2,5,7-trioxa-6,8-diphosphaoct-1-yl)-9H-purin-6-yl]amino]-1-oxopropyl]amino]hexyl]-, P,P'-dioxide

MF C20 H32 N8 O12 P2

CI COM

SR CA

PAGE 1-A



PAGE 1-B

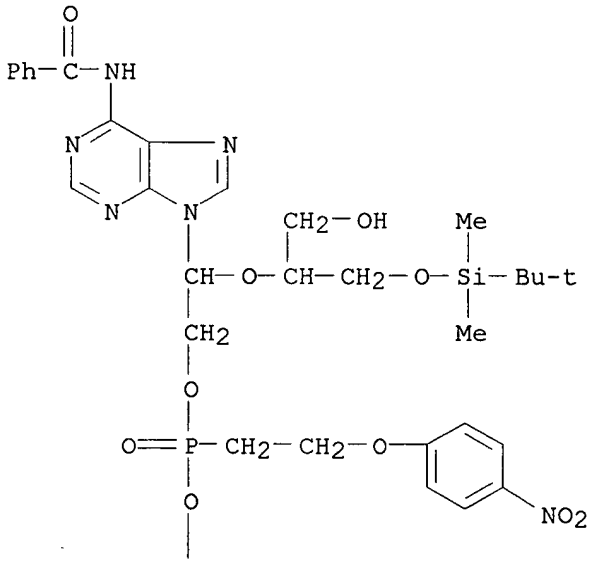
—OPO_3H_2

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

Searched by: Mary Hale 308-4258 CM-1 1E01

L18 ANSWER 15 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 98815-97-5 REGISTRY
CN Phosphoric acid, 2-[1-[6-(benzoylamino)-9H-purin-9-yl]-2-(benzoyloxy)ethoxy]-3-(benzoyloxy)propyl 2,10-bis[6-(benzoylamino)-9H-purin-9-yl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-12-(hydroxymethyl)-7-[2-(4-nitrophenyl)ethyl]-15,15,16,16-tetramethyl-7-oxido-3,6,8,11,14-pentaoxa-7-phospha-15-silaheptadec-1-yl 2-(4-nitrophenyl)ethyl ester, stereoisomer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phosphoric acid, 2-[1-[6-(benzoylamino)-9H-purin-9-yl]-2-(benzoyloxy)ethoxy]-3-(benzoyloxy)propyl 2,10-bis[6-(benzoylamino)-9H-purin-9-yl]-4-[[[(1,1-dimethylethyl)dimethylsilyl]oxy]methyl]-12-(hydroxymethyl)-7-[2-(4-nitrophenyl)ethyl]-15,15,16,16-tetramethyl-3,6,8,11,14-pentaoxa-7-phospha-15-silaheptadec-1-yl 2-(4-nitrophenyl)ethyl ester, P-oxide, stereoisomer
MF C93 H105 N17 O25 P2 Si2
SR CA
LC STN Files: CA, CAPLUS, CASREACT

PAGE 1-A



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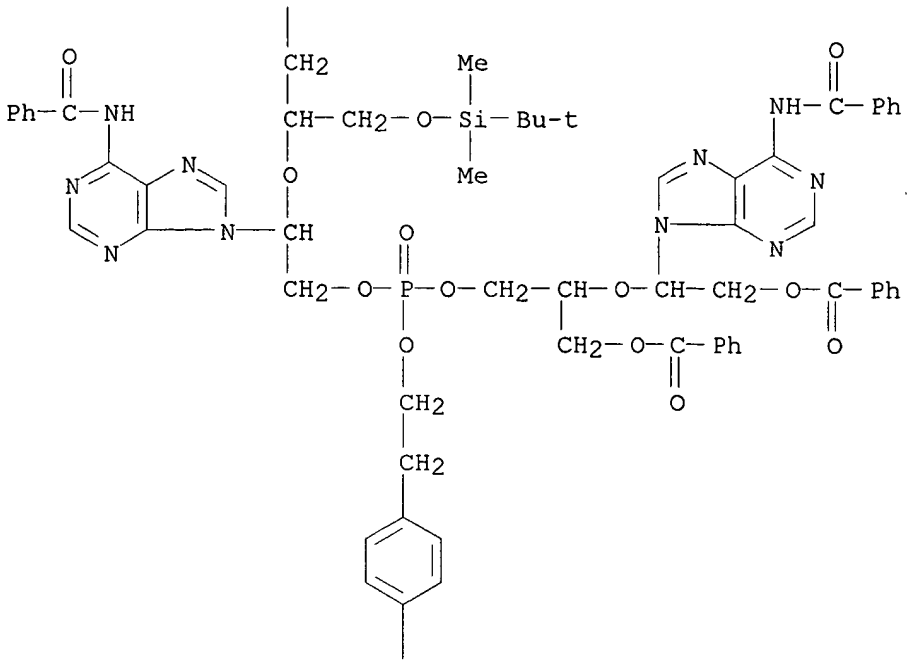


PAGE 3-A

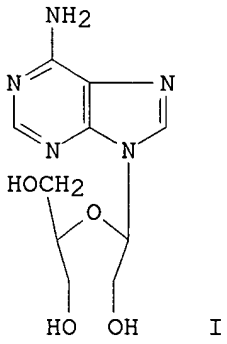
PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 103:178558 Synthesis of a new class of acyclic 2',5'- and 3',5'-oligonucleotide analogs based on 9-[1,5-dihydroxy-4-(S)-hydroxymethyl-3-oxapent-2(R)-yl]adenine. Mikhailov, S. N.; Pfleiderer, Wolfgang (Inst. Mol. Biol., Moscow, B-334, USSR). Tetrahedron Letters, 26(17), 2059-62 (English) 1985. CODEN: TELEAY. ISSN: 0040-4039.

GI

Searched by: Mary Hale 308-4258 CM-1 1E01



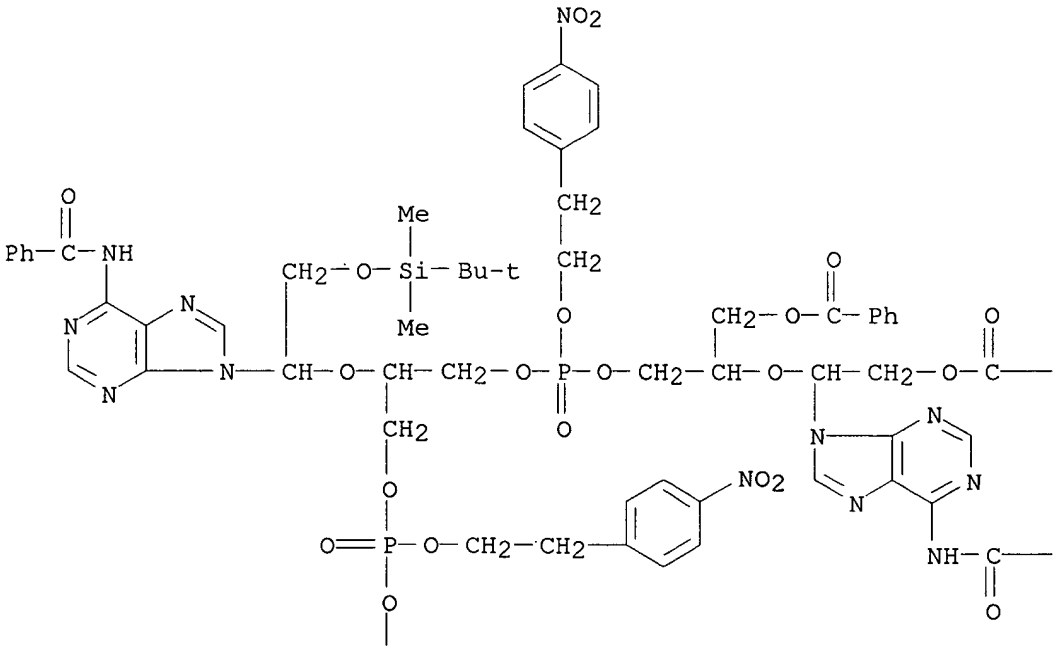
I

AB The acyclic analogs of 2',5'- and 3',5'-oligoadenylates possessing all functional groups of the natural compds. were prepd. on the basis of "oxidized-reduced" adenosine (I).

L18 ANSWER 16 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 98815-96-4 REGISTRY
CN Phosphoric acid, 10-[6-(benzoylamino)-9H-purin-9-yl]-2-[1-[6-(benzoylamino)-9H-purin-9-yl]-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethoxy]-8-[(benzoyloxy)methyl]-5-[2-(4-nitrophenyl)ethoxy]-5-oxido-13-oxo-13-phenyl-4,6,9,12-tetraoxa-5-phosphatridec-1-yl 2-[1-[6-(benzoylamino)-9H-purin-9-yl]-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethoxy]-3-hydroxypropyl 2-(4-nitrophenyl)ethyl ester, stereoisomer (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Phosphoric acid, 10-[6-(benzoylamino)-9H-purin-9-yl]-2-[1-[6-(benzoylamino)-9H-purin-9-yl]-2-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethoxy]-8-[(benzoyloxy)methyl]-5-[2-(4-nitrophenyl)ethoxy]-13-oxo-13-phenyl-4,6,9,12-tetraoxa-5-phosphatridec-1-yl 2-[1-[6-(benzoylamino)-9H-purin-9-yl]-3-[[(1,1-dimethylethyl)dimethylsilyl]oxy]ethoxy]-3-hydroxypropyl 2-(4-nitrophenyl)ethyl ester, P-oxide, stereoisomer
MF C93 H105 N17 O25 P2 Si2
SR CA
LC STN Files: CA, CAPLUS, CASREACT

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A

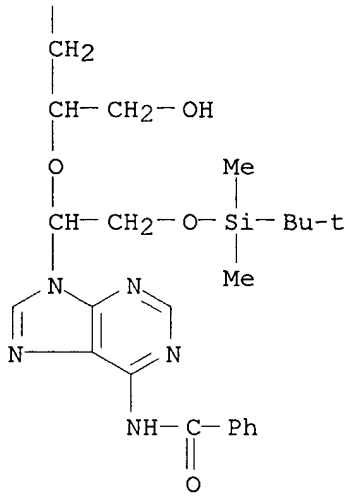


PAGE 1-B

— Ph

— Ph

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 103:178558 Synthesis of a new class of acyclic 2',5'- and 3',5'-oligonucleotide analogs based on 9-[1,5-dihydroxy-4-(S)-hydroxymethyl-3-oxapent-2(R)-yl]adenine. Mikhailov, S. N.; Pfleiderer, Wolfgang (Inst. Mol. Biol., Moscow, B-334, USSR). Tetrahedron Letters, 26(17), 2059-62 (English) 1985. CODEN: TELEAY. ISSN: 0040-4039.

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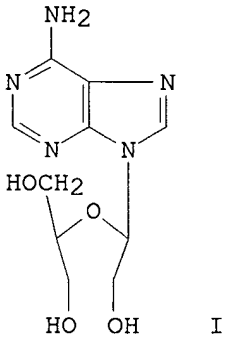

I

AB The acyclic analogs of 2',5'- and 3',5'-oligoadenylates possessing all functional groups of the natural compds. were prepd. on the basis of "oxidized-reduced" adenosine (I).

L18 ANSWER 17 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 82339-88-6 REGISTRY
CN .beta.-Alanine, N-[8-bromo-9-(1,3-diformyl-6,8,8-trihydroxy-6,8-dioxido-2,5,7-trioxa-6,8-diphosphaoct-1-yl)-9H-purin-6-yl]-, [R-(R*,R*)]- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:

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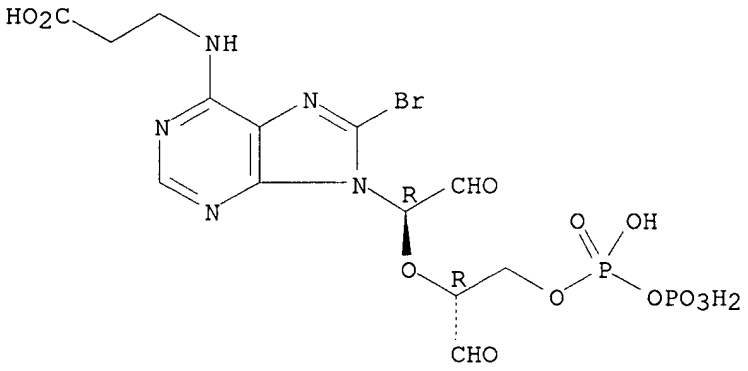
CN .beta.-Alanine, N-[8-bromo-9-(1,3-diformyl-6,8,8-trihydroxy-2,5,7-trioxa-6,8-diphosphaoct-1-yl)-9H-purin-6-yl]-, P,P'-dioxide, [R-(R*,R*)]-
FS STEREOSEARCH
MF C13 H16 Br N5 O12 P2
LC STN Files: CA, CAPLUS

Absolute stereochemistry.



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 97:106259 Enzyme immobilization. (Unitika Ltd., Japan). Jpn. Kokai Tokkyo Koho JP 57039783 A2 19820305 Showa, 5 pp. (Japanese). CODEN: JKXXAF. APPLICATION: JP 1980-115633 19800821.

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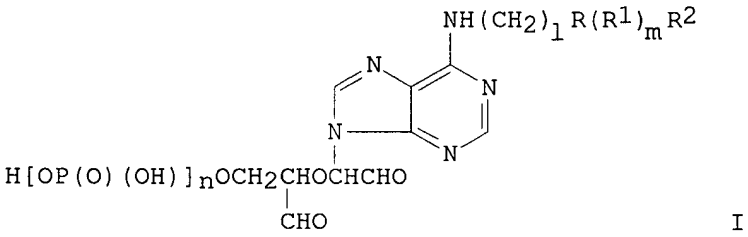

I

AB A substrate for enzyme immobilization, I, consists of an adenosine deriv. in which R is CONH or CO2, R1 is alkyl, arom., or cycloalkyl, and R2 is a high-mol.-wt. support; l = 1 or 2, m = 0 or 1, and n = 1-3. Thus, 5 g Sepharose 4B was swelled in H2O, activated with CNBr, and suspended in 0.1M NaHSO3. 8-Bromo-N6-carboxyethyl-ADP (200 mg) was added and allowed to react for 12 h at 4.degree.. The gel was then washed, resuspended in 50 mL H2O, and treated with 6 mL 0.5M Na metaperiodate for 1 h at room temp. The treated gel with its ribose 2',3'-dialdehyde deriv. of ADP as a substituent was then washed, suspended in 50 mL 0.1M phosphate buffer, pH 8.5, and mixed with 10 mL of a soln. of Bacillus stearothermophilus acetate kinase in the same buffer. The support immobilized 61,000 of 100,000 units applied; a sample of CH-Sepharose 4B taken for comparison immobilized only 4,000 of 20,000 units applied.

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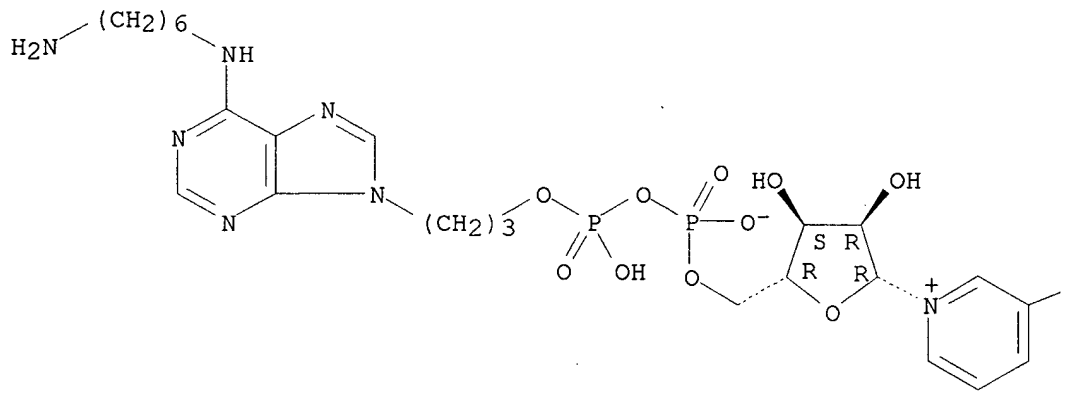
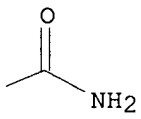
L18 ANSWER 18 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 66443-33-2 REGISTRY
CN Pyridinium, 3-(aminocarbonyl)-1-[5-O-[7-[9-[(6-aminohexyl)amino]-9H-purin-9-yl]-1,3-dihydroxy-1,3-dioxido-2,4-dioxa-1,3-diphosphahept-1-yl]-.beta.-D-ribofuranosyl]-, inner salt (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Pyridinium, 3-(aminocarbonyl)-1-[5-O-[7-[9-[(6-aminohexyl)amino]-9H-purin-9-yl]-1,3-dihydroxy-2,4-dioxa-1,3-diphosphahept-1-yl]-.beta.-D-ribofuranosyl]-, inner salt, P,P'-dioxide
FS STEREOSEARCH
MF C25 H38 N8 O11 P2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

PAGE 1-A



PAGE 1-B

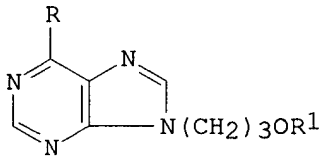


1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

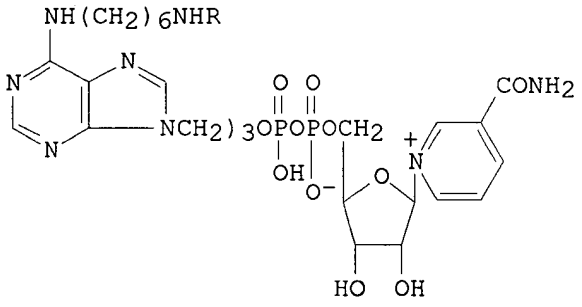
REFERENCE 1: 88:185183 The coenzyme analog (3-[6-(6-aminohexylamino)-9-purinyl]propyl)(nicotinamide-D-ribose)diphosphate as ligand for affinity chromatography of dehydrogenases. Berariu, Veronica; Jeck, Reinhard; Woenckhaus, Christoph (Gustav-Embden-Zent. Biol. Chem., Univ. Frankfurt, Frankfurt/Main, Ger.). Justus Liebigs Ann. Chem. (1), 118-23 (German) 1978. CODEN: JLACBF. ISSN: 0075-4617.

Searched by: Mary Hale 308-4258 CM-1 1E01

GI



I, R=NH(CH2)6NHCOCF3, R1=P(O)(OH)2
II, R=Cl, R1=H



III, R=COCF3
IV, R=H

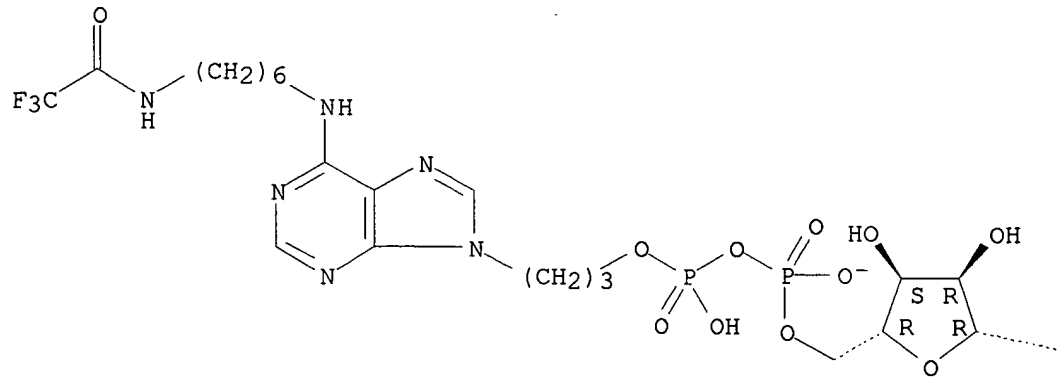
AB 9-[3-(Dihydroxyphosphoryloxy)propyl]-6-[6-(trifluoroacetylamino)hexylamino]-9H-purine (I) was prepd. starting from 6-chloro-9-(3-hydroxypropyl)-9H-purine (II). After condensation of this AMP-analog with dicyclohexylcarbodiimide and NMN in aq. pyridine, a new NAD-analog was formed. The coenzyme analog (3-[6-(6-trifluoroacetylaminohexylamino)-9-purinyl]propyl)(nicotinamide-D-ribose)diphosphate (III) acted as H acceptor (its reduced form as H donor) when tested against different dehydrogenases. Highly dissocd. complexes between this coenzyme analog and dehydrogenases were formed. Removal of the trifluoroacetyl group led to the unstable coenzyme analog (3-[6-(6-aminohexylamino)-9-purinyl]propyl)(nicotinamide-D-ribose)diphosphate (IV), which can be covalently attached to agarose activated with CNBr. When dehydrogenases were applied to the column of the immobilized AMP and NAD-analogs, only glyceraldehyde 3-phosphate dehydrogenase was retained. Elution of the enzyme occurred only after addn. of KCl to the eluant.

L18 ANSWER 19 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 66443-32-1 REGISTRY
CN Pyridinium, 3-(aminocarbonyl)-1-[5-O-[hydroxy[[hydroxy[3-[6-[[6-[(trifluoroacetyl)amino]hexyl]amino]-9H-purin-9-yl]propoxy]phosphinyl]oxy]phosphinyl]-.beta.-D-ribofuranosyl]-, inner salt (9CI) (CA INDEX NAME)
FS STEREOSEARCH
MF C27 H37 F3 N8 O12 P2
LC STN Files: BEILSTEIN*, CA, CAPLUS
(*File contains numerically searchable property data)

Absolute stereochemistry.

Searched by: Mary Hale 308-4258 CM-1 1E01

PAGE 1-A



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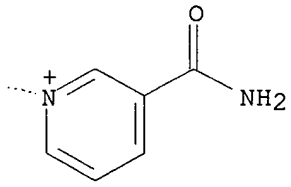

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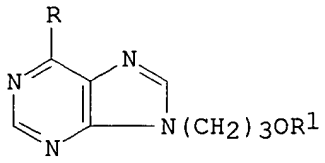
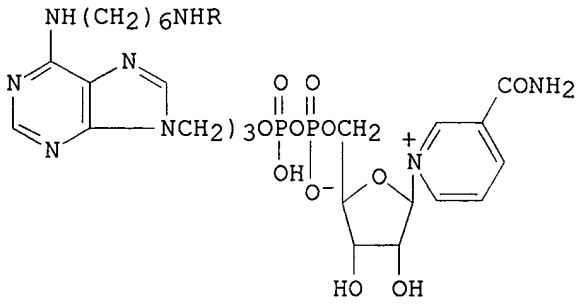
Searched by: Mary Hale 308-4258 CM-1 1E01



I, R=NH(CH2)6NHCOCF3, R1=P(O)(OH)2
II, R=Cl, R1=H

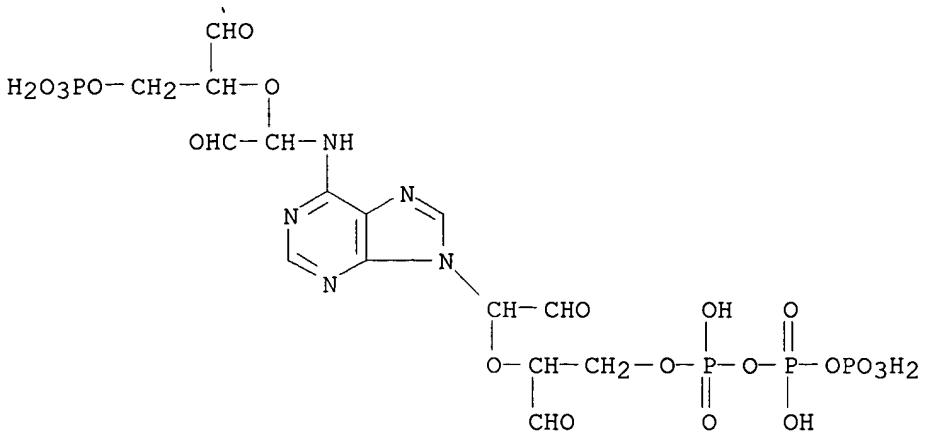


III, R=COCF3
IV, R=H

AB 9-[3-(Dihydroxyphosphoryloxy)propyl]-6-[6-(trifluoroacetylamino)hexylamino]-9H-purine (I) was prepd. starting from 6-chloro-9-(3-hydroxypropyl)-9H-purine (II). After condensation of this AMP-analog with dicyclohexylcarbodiimide and NMN in aq. pyridine, a new NAD-analog was formed. The coenzyme analog (3-[6-(6-trifluoroacetylaminohexylamino)-9-purinyl]propyl)(nicotinamide-D-ribose)diphosphate (III) acted as H acceptor (its reduced form as H donor) when tested against different dehydrogenases. Highly dissocd. complexes between this coenzyme analog and dehydrogenases were formed. Removal of the trifluoroacetyl group led to the unstable coenzyme analog (3-[6-(6-aminohexylamino)-9-purinyl]propyl)(nicotinamide-D-ribose)diphosphate (IV), which can be covalently attached to agarose activated with CNBr. When dehydrogenases were applied to the column of the immobilized AMP and NAD-analogs, only glyceraldehyde 3-phosphate dehydrogenase was retained. Elution of the enzyme occurred only after addn. of KCl to the eluant.

L18 ANSWER 20 OF 20 REGISTRY COPYRIGHT 2002 ACS
RN 56475-05-9 REGISTRY
CN Triphosphoric acid, P-[2-[1-[6-[[1-[1-formyl-2-(phosphonooxy)ethoxy]-2-oxoethyl]amino]-9H-purin-9-yl]-2-oxoethoxy]-3-oxopropyl] ester, stereoisomer (9CI) (CA INDEX NAME)
MF C15 H21 N5 O20 P4
LC STN Files: CA, CAPLUS

Searched by: Mary Hale 308-4258 CM-1 1E01



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 83:93004 Stereochemical course of the adenosine triphosphate phosphoribosyltransferase reaction in histidine biosynthesis. Chelsky, Daniel; Parsons, Stanley M. (Dep. Chem., Univ. California, Santa Barbara, Calif., USA). J. Biol. Chem., 250(14), 5669-73 (English) 1975. CODEN: JBCHA3.

AB The product of the 1st reaction in histidine biosynthesis was shown by optical rotation measurements on 3 derivs. to have inverted, .beta. stereochem. at the newly formed bond. This is in contrast to .alpha. linkage expected on the basis of previously obsd. exchange, specificity, and covalent intermediate phenomena. The postulated double displacement mechanism for ATP phosphoribosyltransferase (EC 2.4.2.17) must be modified to account for the product stereochem.

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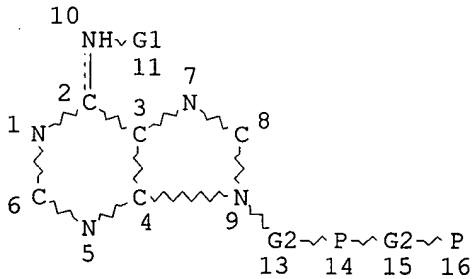

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REP G2=(0-20) A
NODE ATTRIBUTES:

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CONNECT IS E2 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE
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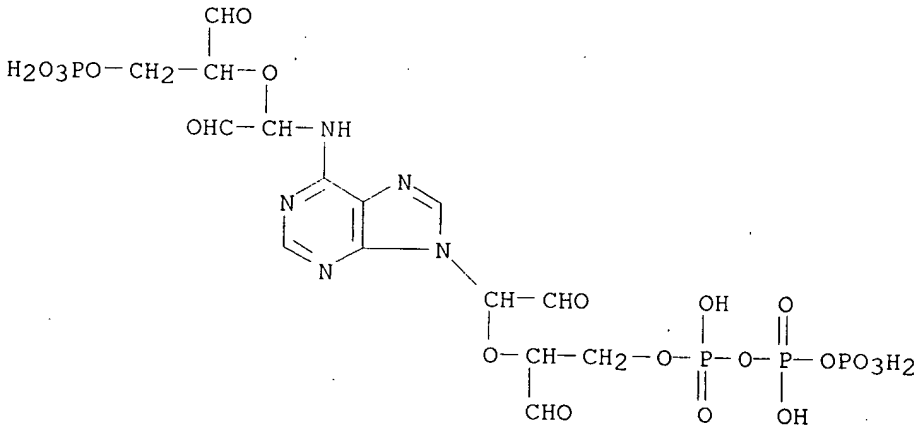
L20 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2002 ACS
RN 56475-05-9 REGISTRY
CN Triphosphoric acid, P-[2-[1-[6-[[1-[1-formyl-2-(phosphonooxy)ethoxy]-2-oxoethyl]amino]-9H-purin-9-yl]-2-oxoethoxy]-3-oxopropyl] ester, stereoisomer (9CI) (CA INDEX NAME)
MF C15 H21 N5 O20 P4
LC STN Files: CA, CAPLUS



PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

1 REFERENCES IN FILE CA (1962 TO DATE)
1 REFERENCES IN FILE CAPLUS (1962 TO DATE)

REFERENCE 1: 83:93004 Stereochemical course of the adenosine triphosphate phosphoribosyltransferase reaction in histidine biosynthesis. Chelsky, Daniel; Parsons, Stanley M. (Dep. Chem., Univ. California, Santa Barbara, Calif., USA). J. Biol. Chem., 250(14), 5669-73 (English) 1975. CODEN: JBCHA3.

AB The product of the 1st reaction in histidine biosynthesis was shown by optical rotation measurements on 3 derivs. to have inverted, .beta. stereochem. at the newly formed bond. This is in contrast to .alpha.

Searched by: Mary Hale 308-4258 CM-1 1E01

linkage expected on the basis of previously obsd. exchange, specificity, and covalent intermediate phenomena. The postulated double displacement mechanism for ATP phosphoribosyltransferase (EC 2.4.2.17) must be modified to account for the product stereochem.

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  more information.


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L8          259433 SEARCH L7
L9                  SCR 2017
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Searched by: Mary Hale 308-4258 CM-1 1E01

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